

Simple Step-by-Step Guides to Solving Chemistry Problems

Determining Empirical & Molecular Formula



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Calculating Empirical & Molecular Formula

Chemical formula spells out the composition of chemical compounds and even the way in which the atoms are arranged using a single line of chemical element symbols, numbers, and other symbols, such as dashes, commas, brackets, and plus (+) and minus (-) signs. There are several types of chemical formula. These include empirical formula, molecular (or true) formulas, and structural formulas.

Molecular formulas have relative formula masses that are whole-number multiples (n) of the corresponding *empirical relative formula mass*. Chemical compounds with the empirical formula CH_2O (relative formula mass = 30) will have a relative formula mass which is a multiple of 30, ie $\text{C}_2\text{H}_4\text{O}_2$ (RFM = 60), $\text{C}_2\text{H}_6\text{O}_3$ (RFM = 90), $\text{C}_{10}\text{H}_{20}\text{O}_{10}$ (RFM = 300).

Empirical Formula from Molecular Formula, $\text{X}_a\text{Y}_b\text{Z}_c$

Step 1: Write down the subscripts, ie a, b, c ;

Step 2: Identify the largest number that divides into a, b and c ;

Step 3: Divide all subscripts by the number identified in step 2;

Step 4: Write down the empirical formula.

Example: What is the empirical formula of $\text{C}_6\text{H}_{12}\text{O}_6$?

Step 1	Write down chemical formula subscripts	6, 12, 6
Step 2	Identify the largest common factor	6
Step 3	Divide subscripts by the largest common factor	$\text{C}_{6/6} \text{H}_{12/6} \text{O}_{6/6}$
Step 4	Write down the empirical formula	Empirical Formula: CH_2O

Example: What is the empirical formula of $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$?

Step 1	Write down chemical formula subscripts	8, 10, 4, 2
Step 2	Identify the largest common factor	2
Step 3	Divide subscripts by the largest common factor	$\text{C}_{8/2} \text{H}_{10/2} \text{N}_{4/2} \text{O}_{2/2}$
Step 4	Write down the empirical formula	Empirical Formula: $\text{C}_4 \text{H}_5 \text{N}_2 \text{O}$

Empirical Formula from % Composition

To calculate empirical formula from percentage compositions of a compound use the calculating frame given below:

Empirical Formula from Percentage Composition Calculating Frame

Step 1: Write the names or symbols of the elements;

Step 2: For each element give its % composition;

Step 3: Using the Periodic Table find the A_r value for each element;

Step 4: Divide the % value for each element by its A_r ;

Step 5: Divide throughout by the smallest value;

Step 6: Write down the empirical formula.

The action at Step 5 usually gives you the simplest whole number ratio straightaway. Sometimes it does not, so you might get 1 and 1.5. In this example, you would multiply both numbers by 2, giving 2 and 3 (instead of rounding 1.5 up to 2).

Step 1		Element X	Element Y	Element Z
Step 2	% composition	x	y	z
Step 3	Relative atomic mass, A_r	$A_r[X]$	$A_r[Y]$	$A_r[Z]$
Step 4	% composition/ $A_r \times 100$	$x/A_r[X] \times 100$	$y/A_r[Y] \times 100$	$z/A_r[Z] \times 100$
Step 5	Divide by smallest number from Step 4	Step 4 answer/ Smallest no. Step 4 = a	Step 4 answer/ Smallest no. Step 4 = b	Step 4 answer/ Smallest no. Step 4 = c
Step 6	Empirical Formula	$X_aY_bZ_c$		

Example: What is the empirical formula of the nitrogen oxide that has 30.4% by mass nitrogen and 69.6% by mass oxygen?

Answer:

Step 1		N	O
Step 2	% composition	30.4	69.6
Step 3	A_r	14	16
Step 4	% composition/ A_r	$30.4/14 = 2.17$	$69.6/16 = 4.35$
Step 5	Divide by small number from step 4	$2.17/2.17 = 1$	$4.35/2.17 = 2$
Step 6	Empirical Formula:	N₂O	

Empirical Formula: N₂O

Example: What is the empirical formula of a compound was found to contain 32.65% sulfur, 65.3% oxygen and 2.04% hydrogen?

Answer:

Step 1		S	O	H
Step 2	% composition	32.65	65.3	2.04

Step 3	A_r	32	16	1
Step 4	% composition/ A_r	$32.65/32 = 1.02$	$65.3/16 = 4.08$	$2.01/1 = 2.01$
Step 5	Divide by small number from step 4	$1.02/1.02 = 1$	$4.08/1.02 = 4$	$2.01/1.02 = 2$
Step 6	Empirical Formula	SO_4H_2		

Empirical formula: H_2SO_4

Empirical Formula from Elemental Masses (XYZ)

If you are given the elemental composition of an unknown substance in grams, you will need to proceed according to the following instructions.

Example: Find the empirical formula of an unknown substance made from p grams of element X, q grams of element Y and r grams of element Z.

- Step 1:** Write the names or symbols of the elements;
- Step 2:** Determine total mass of unknown substance, i.e. $p + q + r$ grams
- Step 3:** For each element calculate its % composition, i.e. $p/(p + q + r) \times 100$
- Step 4:** Using the Periodic Table find the A_r value for each element;
- Step 5:** Divide the % value for each element calculated in Step 3 by its A_r ;
- Step 6:** Divide throughout by the smallest value calculated in Step 5;
- Step 7:** Write down the empirical formula.

Step 1		X	Y	Z	Total
Step 2	Mass	n	p	q	$x + y + z$
Step 3	% Composition	$p/(p + q + r) \times 100$	$q/(p + q + r) \times 100$	$r/(p + q + r) \times 100$	
Step 4	A_r	$A_r[X]$	$A_r[Y]$	$A_r[Z]$	
Step 5	Divide step 2 value for each element by its A_r	Step 2 value/ $A_r[X]$	Step 2 value/ $A_r[Y]$	Step 2 value/ $A_r[Z]$	
Step 6	Divide Step 4 answer by the lowest step 4 value	Step 4 value/Lowest Step 4 value = a	Step 4 value/Lowest Step 4 value = b	Step 4 value/Lowest Step 4 value = c	
Step 7	Empirical Formula	$X_aY_bZ_c$			

Answer:

A compound of was found to contain 4g of mercury and 0.64 g of sulfur. What is

Step 1		Hg	S	Total
Step 2	Mass	4	0.64	4.64
Step 3	% composition	$4/4.64 \times 100 = 86.2$	$0.64/4.64 \times 100 = 13.8$	

Step 4	A_r	200.6	32	
Step 5	% composition/ A_r	$86.2/200.6 \times 100 = 0.43$	$13.8/32 \times 100 = 0.43$	
Step 6	Ratio	$0.43/0.43 = 1$	$0.43/0.43 = 1$	
Step 7	Empirical Formula	HgS		

Molecular Formula from Empirical Formula

Step 1: Calculate the relative empirical formula mass.

Step 2: Divide the relative molecular formula mass by relative empirical formula mass. You should get a whole number (n).

Step 3: Multiply each of the subscripts within the empirical formula by the number calculated (n) in Step 2 to obtain the molecular formula.

Example: Naphthalene is a carbon and hydrogen containing compound often used in moth balls. The empirical formula is C_5H_4 and its molar mass is 128.16g/mol. Find its molecular formula.

Step 1: Empirical Formula Mass = $(12 \times 5) + (1 \times 4) = 74$

Step 2: $n = \text{Molecular Formula Mass} / \text{Empirical Formula Mass} = 128/74 = 2$

Step 3: Molecular Formula = $2 \times \text{empirical formula} = C_{(5 \times 2)} H_{(4 \times 2)}$
 $= C_{10}H_8$

Example: A compound containing 40.0% carbon, 5.7% hydrogen and 53.3% oxygen has an atomic mass of 175 g/mol. What is the molecular formula?

Step 1		C	H	O
Step 2	% composition	40	5.7	53.3
Step 3	A_r	12	1	16
Step 4	% composition/ A_r	$40/12$	$5.7/1$	$53.3/16$
Step 5	Ratio	3.33	5.7	3.33
		1	1.67	1
Step 6	Empirical Formula			

? Practice Problems

- What is the empirical formula of the following compounds?
 - C_6H_6

- b. C_8H_{18}
 - c. CO_2
 - d. $C_2H_6O_2$
 - e. $X_{39}Y_{13}$
2. A 15.0g sample of a compound was found to contain 8.83g sodium and 6.17g sulfur. Calculate the empirical formula of this compound.
 3. Analysis of a 10.150g sample of a compound known to contain only phosphorus and oxygen indicates a phosphorus content of a 4.433g. What is the empirical formula of this compound.
 4. A sample of an oxide of arsenic is found to contain 75.74% arsenic. What is its empirical formula?
 5. What is the empirical formula for a compound containing 26.57% potassium, 35.36% chromium, and 38.07% oxygen?
 6. What is the empirical and molecular formulas of Ibuprofen which has a mass composition of 75.69% C, 8.80% H and 15.51% O and the molecular mass is approximately 206 g/mol. $C_{13}H_{18}O_2$.
 7. Epsom salts, a strong laxative used in veterinary medicine, is a hydrate. The formula for Epsom salts can be written as $MgSO_4 \cdot xH_2O$, where x indicates the moles of water for every mole of magnesium sulfate. When 5.061 g of this hydrate is heated to 250°C, all the water of hydration is lost, leaving 2.472 g of $MgSO_4$. What is the value of x?
 8. When 2.5000 g of an oxide of mercury, (Hg_xO_y) is decomposed into the elements by heating, 2.405 g of mercury are produced. Calculate the empirical formula.
 9. The compound benzamide has the following percent composition. What is the empirical formula?
C = 69.40 % H= 5.825 % O = 13.21 % N= 11.57 %
 10. Nicotine, an alkaloid in the nightshade family of plants that is mainly responsible for the addictive nature of cigarettes, contains 74.02% C, 8.710% H, and 17.27% N. If 40.57 g of nicotine contains 0.2500 mole nicotine, what is the molecular formula?

Answers are given on the next page.

? Practice Problem Answers

1. What is the empirical formula of the following compounds?

a. C_6H_6

Step 1	Write down chemical formula subscripts	6, 6
Step 2	Identify the largest common factor	6
Step 3	Divide subscripts by the largest common factor	$C_{6/6} H_{6/6}$
Step 4	Write down the empirical formula	Empirical Formula: CH

b. C_8H_{18}

Step 1	Write down chemical formula subscripts	8, 18
Step 2	Identify the largest common factor	2
Step 3	Divide subscripts by the largest common factor	$C_{8/2} H_{18/2}$
Step 4	Write down the empirical formula	Empirical Formula: C_4H_9

c. CO_2

Step 1	Write down chemical formula subscripts	1, 2
Step 2	Identify the largest common factor	1
Step 3	Divide subscripts by the largest common factor	$C_{1/1} O_{2/1}$
Step 4	Write down the empirical formula	Empirical Formula: CO_2

d. $C_2H_6O_2$

Step 1	Write down chemical formula subscripts	2, 6, 2
Step 2	Identify the largest common factor	2
Step 3	Divide subscripts by the largest common factor	$C_{2/2} H_{6/2} O_{2/2}$
Step 4	Write down the empirical formula	Empirical Formula: CH_3O

e. $X_{39}Y_{13}$

Step 1	Write down chemical formula subscripts	13, 29
Step 2	Identify the largest common factor	13
Step 3	Divide subscripts by the largest common factor	$X_{39/13} Y_{13/13}$
Step 4	Write down the empirical formula	Empirical Formula: X_3Y

2. A 15.0g sample of a compound was found to contain 8.83g sodium and 6.17g sulfur. Calculate the empirical formula of this compound.

Answer

Step 1		Na	S	Total
Step 2	Mass	8.83	6.17	15.0
Step 3	% composition	$8.83/15 \times 100 = 58.9$	$6.17/15 \times 100 = 41.1$	
Step 4	A_r	23	32	
Step 5	% composition/ A_r	$58.9/23$	$41.1/32$	

Step 6	Ratio	2.56 2	1.28 1	
Step 7	Empirical Formula	Na₂O		

3. Analysis of a 10.150g sample of a compound known to contain only phosphorus and oxygen indicates a phosphorus content of a 4.433g. What is the empirical formula of this compound.

Step 1		P	O	Total
Step 2	Mass	4.433	10.15-4.433 = 5.717	10.15
Step 3	% composition	4.433/10.15 x 100 = 43.7	5.717/10.15 x 100 = 56.3	
Step 4	A _r	31	16	
Step 5	% composition/A _r	43.7/31 = 1.4	56.3/16 = 3.52	
Step 6	Ratio	1 2	2.5 5	
Step 7	Empirical Formula	P₂O₅		

4. A sample of an oxide of arsenic is found to contain 75.74% arsenic. What is its empirical formula?

Step 1		As	O
Step 2	% composition	75.74	100 - 75.74 = 24.26
Step 3	A _r	75	16
Step 4	% composition/A _r	75.74/75 = 1	24.26/16 x 100 = 1.5
Step 5	Ratio	1 2	1.5 3
Step 6	Empirical Formula	As₂O₃	

5. What is the empirical formula for a compound containing 26.57% potassium, 35.36% chromium, and 38.07% oxygen?

Step 1		K	Cr	O
Step 2	% composition	26.57	35.36	38.07
Step 3	A _r	39	52	16
Step 4	% composition/A _r	26.57/39 = 0.68	35.36/52 = 0.68	38.07/16 = 2.38
Step 5	Ratio	1	1	4
Step 6	Empirical Formula	KCrO₄		

6. What is the empirical and molecular formulas of Ibuprofen which has a mass composition of 75.69% C, 8.80% H and 15.51% O and the molecular mass is approximately 206 g/mol.

Step 1		C	H	O
Step 2	% composition	75.69	8.8	15.51
Step 3	A _r	12	1	16
Step 4	% composition/A _r	6.3	8.8	0.97

Step 5	Ratio	6.5 13	9 18	1 2
Step 6	Empirical Formula	C₁₃H₁₈O₂		

$$\text{RFM}[\text{C}_{13}\text{H}_{18}\text{O}_2] = 206$$

7. Epsom salts, a strong laxative used in veterinary medicine, is a hydrate. The formula for Epsom salts can be written as $\text{MgSO}_4 \cdot x\text{H}_2\text{O}$, where x indicates the moles of water for every mole of magnesium sulfate. When 5.061 g of this hydrate is heated to 250°C , all the water of hydration is lost, leaving 2.472 g of MgSO_4 . What is the value of x ?

	$\text{MgSO}_4 \cdot x\text{H}_2\text{O}$	$\text{MgSO}_4 + x\text{H}_2\text{O}$		
Step 1		$\text{MgSO}_4 \cdot x\text{H}_2\text{O}$	MgSO_4	H_2O
Step 2	Mass	5.061	2.472	$5.061 - 2.472 = 2.589$
Step 3	% composition	5.061	$2.472/5.061 \times 100 = 48.84$	$2.589/5.061 \times 100 = 51.15$
Step 4	M_r	$120 + 18x$	120	18
Step 5	% composition/ M_r		$48.84/120 = 0.41$	$51.15/18 = 2.84$
Step 6	Ratio		1	7
	Formula	MgSO₄·7H₂O		

8. When 2.5000 g of an oxide of mercury, (Hg_xO_y) is decomposed into the elements by heating, 2.405 g of mercury are produced. Calculate the empirical formula.

Step 1		Hg	O	Total
Step 2	Mass	2.405	$2.500 - 2.405 = 0.095$	2.500
Step 3	% composition	$2.405/2.5 \times 100 = 96.2$	$0.095/2.500 \times 100 = 3.8$	
Step 4	A_r	200.6	16	
Step 5	% composition/ A_r	$96.2/200.6 = 0.48$	$3.8/16 = 0.24$	
Step 6	Ratio	2	1	
Step 7	Empirical Formula	Hg₂O		

9. The compound benzamide has the following percent composition. What is the empirical formula?
 C = 69.40 % H = 5.825 % O = 13.21 % N = 11.57 %

Step 1		C	H	O	N
Step 2	% composition	69.4	5.825	13.21	11.57
Step 3	A_r	12	1	16	14
Step 4					
Step 5	% composition/ A_r	$69.4/12 =$	$5.825/1 = 5.825$	$13.21/16 =$	$11.57/14 =$
Step 6	Ratio	5.78 7	5.825 7	0.825 1	0.826 1
Step 7	Empirical Formula	C₇H₇NO			

10. Nicotine, an alkaloid in the nightshade family of plants that is mainly responsible for the addictive nature of cigarettes, contains 74.02% C, 8.710% H, and 17.27% N. If 40.57 g of nicotine contains 0.2500 mole nicotine, what is its molecular formula?

Step 1		C	H	N
Step 2	% composition	74.02 =	8.71	17.27
Step 3	A_r	12	1	14
Step 4	% composition/ A_r	$74.02/12 = 6.17$	$8.71/1 = 8.71$	$17.27/14 = 1.23$
Step 5	Ratio	5	7	1
Step 6	Empirical Formula	C₅H₇N		
	Molecular Formula	C₁₀H₁₄N₂		

Empirical Formula RFM[C₅H₇N] = 81

Molecular Mass = mass/no. of moles = $40.57/0.25 = 162$

Molecular Formula = C₁₀H₁₄N₂